

New ^{56}Fe Evaluation for the CIELO project

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Abstract. The Collaborative International Evaluated Library Organisation (CIELO) aims to provide revised and updated evaluations for ^{239}Pu , $^{238,235}\text{U}$, ^{56}Fe , ^{16}O , and ^1H through international collaboration. This work, which is part of the CIELO project, presents the initial results for the evaluation of the ^{56}Fe isotope, with neutron-incident energy ranging from 0 to 20 MeV. The $^{56}\text{Fe}(n,p)$ cross sections were fitted to reproduce the ones from IRDFF dosimetry file. Our preliminary file provides good cross-section agreements for the main angle-integrated reactions, as well as a reasonable overall agreement for angular distributions and double-differential spectra, when compared to previous evaluations.

1 Introduction

The Collaborative International Evaluated Library Organisation (CIELO) is a pilot project from Subgroup 40 of the Working Party on International Nuclear Data Evaluation Co-operation (WPEC - SG40). Its main goal is to test the scheme of a broad international collaboration to produce new evaluated nuclear reaction data files. For this purpose evaluators from across the world will re-evaluate all the six main nuclides for reactor applications: ^{239}Pu , $^{238,235}\text{U}$, ^{56}Fe , ^{16}O , and ^1H . This present work describes efforts to produce an updated file for ^{56}Fe , with special focus on the fast region.

2 Experimental data

There is a great amount of experimental data for ^{56}Fe and also for $^{\text{Nat}}\text{Fe}$, of which 91.72% consists of the mass-56 isotope. To perform this evaluation we referred to careful reviews and previous evaluations, such as Refs. [1–3]. We also took into account recent experimental results [4].

3 Reaction calculations

For the reaction calculations we used the EMPIRE code [5] and for fitting its parameters we employed the KALMAN code, which is part of the EMPIRE package.

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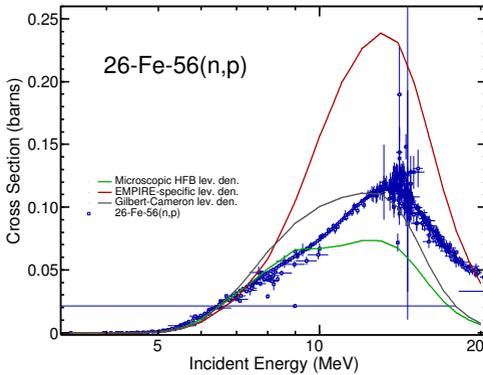


Figure 1. Different results for $^{56}\text{Fe}(n,p)$ cross section obtained by EMPIRE default calculations using different level-density models: microscopic Hartree-Fock-Bogoliubov (green curve); EMPIRE-specific level densities adjusted to RIPL-3 experimental D_{obs} and to discrete levels (red curve); Gilbert-Cameron level-density model (gray curve).

3.1 Models adopted

In this section we will describe the models which were adopted in the calculations leading to the results that will be presented in the following sections.

The coupled channels approach was adopted to describe the direct reaction part, with levels not explicitly coupled being handled through Distorted-Wave Born Approximation (DWBA). The optical model potential used was the ^{56}Fe -specific dispersive potential by Soukhovitskii and Capote [6]. To account for the correlations between incident and exit channels in elastic scattering (width fluctuation correction) the model by Hofmann, Richert, Tepel and Weidenmueller (HRTW) [7] was employed up to incident energy of 8 MeV. The γ strength function adopted was the version 1 of the Modified Lorentzian (MLO1) from Ref. [8]. The pre-equilibrium contribution to neutron emission was treated in terms of the TUL formulation [9] of the multi-step direct mechanism for incident energies above 3 MeV complemented with the NVWY [10] multi-step compound in the whole energy range. The classical exciton model (PCROSS option), with Iwamoto-Harada extension for clusters, was used for the remaining ejectiles. The multiplier on the free path of excitons was set to 2.5. The adopted optical model, while performing superbly at higher incident energies, overshoots experimental data below 3 MeV. To compensate for this deficiency an energy-dependent factor scaling all cross sections was applied up to 3 MeV. We did not attempt a more rigorous approach of refitting parameters of the optical potential since in the final evaluation the region in question will be represented by experimental data.

3.2 Selection of level-density model

The $^{56}\text{Fe}(n,p)$ reaction has been carefully evaluated and extremely well defined for the IRDFF dosimetry file [1]. Calculations show strong sensitivity of the $^{56}\text{Fe}(n,p)$ cross sections to level densities (LD), indicating that this reaction may provide a very stringent test of the employed LD model. In Fig. 1 we show preliminary results obtained by default EMPIRE calculation using three different LD models.

We initially adopted the microscopic HFB LD model for further fitting as it reproduces the observed data in the region below ~ 9 MeV (see Fig. 1) and at higher energies we could manually alter pre-calculated RIPL-3 tables to impose agreement with the IRDFF file. It was observed that (n,p) cross sections depend strongly on both ^{56}Fe (incoming channel) and ^{56}Mn (outgoing channel) LD. After preliminary fittings of ^{56}Mn LD parameters we reached a reasonably good agreement, as seen in Fig. 2(a) (red curve). It is observed that a very minor change in LD, from red to blue curves in Fig. 2(b), already leads to a noticeable change in calculated cross sections (Fig. 2(a)). Moreover, the green curve in Fig. 2(b) represents a fit of the experimental LD measured by Schiller *et al.* [4], which is not dramatically different from the red curve. However, the corresponding cross section (green

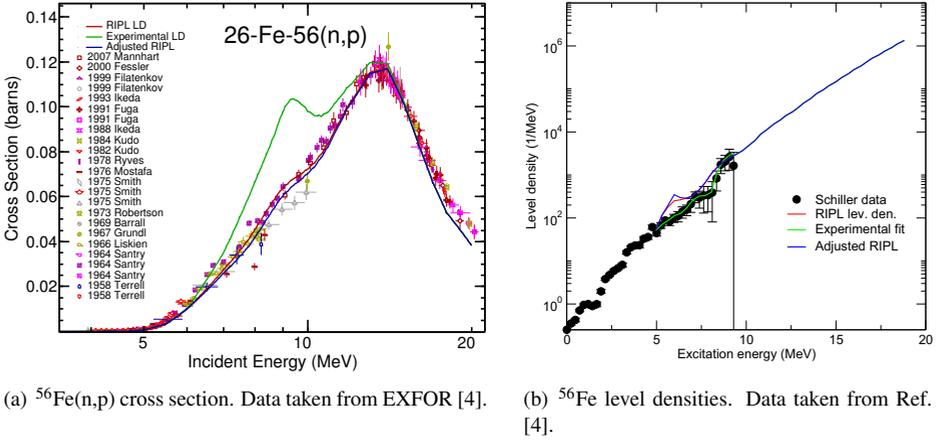


Figure 2. $^{56}\text{Fe}(n,p)$ cross section (left) and the corresponding level density used in calculation (right).

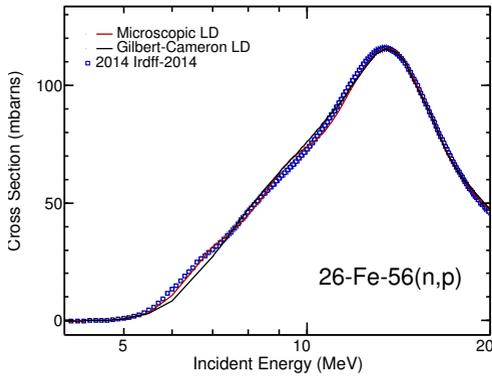
curve in Fig. 2(a)) is in significant disagreement with experimental data. This is likely to be due to different assumptions about spin and parity distributions during processing of the measurements.

Two LD models were selected for further testing: the HFB microscopic model and the Gilbert-Cameron (GC) one. In the case of the former we fitted the pairing-like and pseudo- α parameters for ^{56}Mn , in order to reproduce the IRDFF (n,p) cross section. We also introduced minor changes to the ^{56}Fe LD. In the case of GC model we fitted only the α level density parameter, aiming to reproduce IRDFF (n,p) and experimental α production [4] cross sections. All other LD parameters from GC model were calculated internally to ensure consistency and physically reasonable matching between LD and discrete levels. The energy-dependent tuning of the equilibrium decay width for the α channel was introduced for incident energies between 9 and 18 MeV to account for model deficiencies.

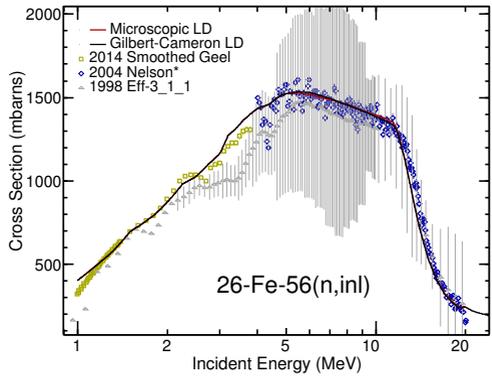
In Fig 3 we present some of the results obtained by our calculations and fits, for both microscopic HFB and Gilbert-Cameron LD models. Fig. 3(a) shows that calculations from both models are in good agreement with IRDFF, even though GC model does not reproduce the region around 6-7 MeV as well the microscopic HFB model. This is understandable in view of the stronger constraints on the GC model in contrast with the arbitrary modifications applied to the HFB model. For the total inelastic (Fig. 3(b)) we can observe a small difference between the results from the two LD models, both in agreement with recent experiments. Fig 3(c) show that GC model leads to slight improvement of the agreement with experimental data of the $^{56}\text{Fe}(n,2n)$ reaction. Additionally, Figs. 3(d) and 3(e) (which correspond to double-differential spectra at 8.17 MeV and α production cross section, respectively) display a significantly better agreement of GC model calculations when compared with the HFB ones.

3.3 Angular distributions

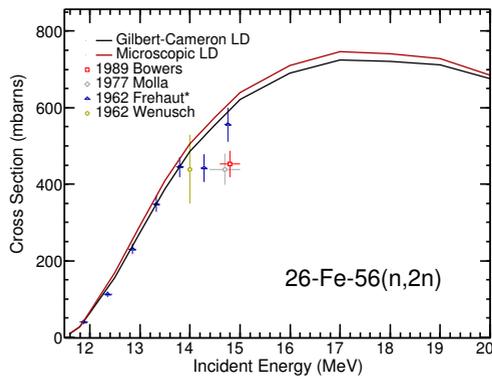
For angular distributions we assembled a full file according to the following prescription. *Integrated cross sections:* Up to 846 keV, which is the threshold for the first inelastic state, the evaluated file consists of fitted resonance parameters. The total cross section, for neutron-incident energy between 846 keV and 4 MeV, is given by JEFF-3.2 [3], which corresponds to smoothed Berthold *et al.* experimental data [4]. Angle-integrated inelastic cross sections for the excited levels are given by experimental data from Negret *et al.* [11]. All other channels, except the elastic one, are taken from EMPIRE calculations with GC LD, as the elastic is defined as the difference between the total cross section and



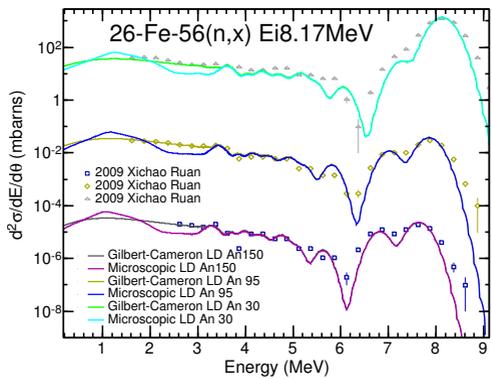
(a) $^{56}\text{Fe}(n,p)$ cross section. Data taken from IRDF [1].



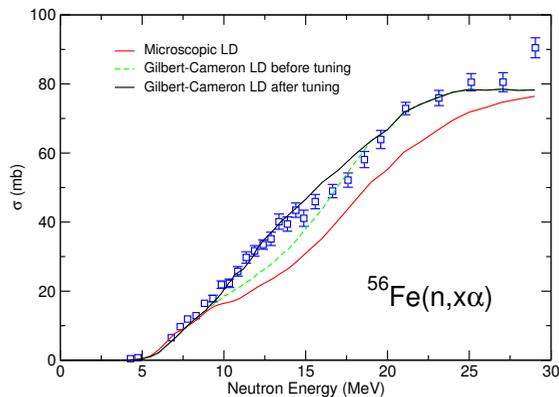
(b) ^{56}Fe inelastic cross section. Data taken from EXFOR [4].



(c) $^{56}\text{Fe}(n,2n)$ cross section. Data taken from EXFOR [4].



(d) ^{56}Fe double-differential spectra at 8.17 MeV for 30, 95 and 150 degrees. A successive factor of 10^3 was applied for the last two angles to facilitate the visualization. Data taken from EXFOR [4].



(e) $^{56}\text{Fe}(n,\alpha)$ cross section. Data taken from Ref. [4].

Figure 3. Comparison of results for both LD models for different neutron-induced reactions on ^{56}Fe .

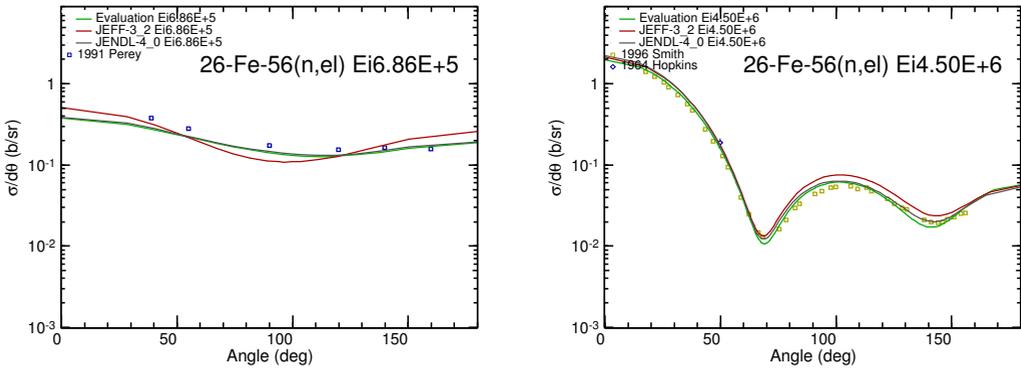


Figure 4. (color online) Elastic angular distributions for neutron-incident energy of 686keV (left panel) and 4.50 MeV (right panel) as examples.

the sum of all other channels. *Angular distributions:* The angular distributions for incident energies lying within the resonance region and up to 846 keV are taken from JENDL-4.0 [2]. For all other values of incident energy, differential cross sections are obtained directly from EMPIRE calculations.

Due to the the large availability of experimental data in the literature we were able to generate more than 2800 elastic angular distribution plots. In Fig. 4 we show as example two of them: one for the lower incident-energy regime and one for a higher energy.

4 Conclusions

In this work we presented the latest developments on a new reaction evaluation for ^{56}Fe , as part of the CIELO project. Calculations show great sensibility of cross sections on the level-density model adopted. Comparisons indicate that employing Gilbert Cameron LD model provides better results. $^{56}\text{Fe}(n,p)$ cross sections were succesfully fitted to the IRDFF dosimetry file while other reaction channels are in good agreement with experimental data. An assembled file was produced with associated elastic angular distributions calculated, reaching reasonably good agreement with experimental data.

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